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An approach to identify the atomic arrangement in nanometer range-size

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Nanostructured materials and particles have received great attention due to various functions and adjustable properties including size and shape [1]. The multi-space structure of nanoparticle including defects and micro-strain determines their physical and chemical properties. The development of analytical method to reveal multi-scale structure in atomic scale is crucial to understanding the properties of particles.

In the present study, we constructed the system to calculate the X-ray diffraction pattern from the atomic arrangement of nano-particle in real space using graphic processing units (GPU). The system calculates the pattern based on the Dybe-Sherrier scattering equation (DSE) [2]. We are developing the analytical method to determine the multi-scale structure which is including the size, defects and strains of the particle in atomic scale.

Figure 1 shows observed experimental data and the calculated profiles of our system. Na1.32Mn[Fe(CN)6]0.833.6H2O (NMF) was used as a target materials. The calculation were carried out using 40nm particle size. We used two kinds of atomic arrangements. One is periodical arrangement of a unit cell called perfect model. Another is the model including the strain called strain model. We created atomic arrangement of particle with strain. We have observed the peak broadening in the profile of the strain model. The profile shape of the strain model shows similar feature of the experimental data of NMF.

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